Renormalized Single-Particle Energies

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Abstract

Using a shell model diagonalization which includes $2\hbar\omega$ excitations the spin-orbit splittings for mass numbers 5, 15 and 17 are studied. The contributions of the two-body spin-orbit and tensor interactions are studied separately and in combination. It is found that the second-order effects involving the two-body spin-orbit interaction are more important than the second-order tensor effects. For $A = 5$, the overall effect of the higher-shell admixtures is to decrease the $p_{1/2} - p_{3/2}$ splitting, but for $A = 15$ this splitting is increased by a fair amount, and for $A = 17$ there is only a miniscule increase in the $d_{3/2} - d_{5/2}$ splitting. These results are in qualitative agreement with data as well as perturbative analysis.

I. INTRODUCTION

In this work we consider how higher shell admixtures affect single-particle energies, especially spin-orbit splittings. This problem is of long-standing interest. For example, we quote from Bohr and Mottelson [1] "Finally, the tensor force contributes in second-order and higher order to the effective one-body spin-orbit potentials". They refer to the 1960 work of Terasawa *et.al* [2,3].

Indeed, in the 1960 works, the authors get a large 'spin-orbit' splitting from the tensor interaction (and of the correct sign), enough to explain a substantial amount if not all of the spin-orbit splitting observed in mass 5 systems. However, Terasawa noted that other groups got very small effects, some even of the opposite sign. One of the main motivations for Terasawa's work [2] was his feeling at that time (*i.e* 1960) that it was not clear that one needed a strong two-body spin-orbit to explain the nucleon-nucleon data. Furthermore, there were some theoretical calculations that supported a very strong tensor interaction. Of course, at the present time, the strong two-body spin-orbit interaction is well established, but we can still ask if the two-body tensor interaction contributes to the one-body spin-orbit splitting in second order.

The problem of the single-particle energies, and in particular the spin-orbit splitting, was adressed more recently for $A = 15$ and $A = 17$ (but not $A = 5$) by Zamick, Zheng and Müther [4]. They used both non-relativistic and relativistic G-matrices derived from the Bonn A and Bonn C interactions, and they used second-order perturbation theory to calculate the $p_{1/2} - p_{3/2}$ hole splitting in $A = 15$ as well as the $d_{3/2} - d_{5/2}$ particle splitting in $A = 17$. They divided the Goldstone diagrams into non Hartree-Fock (NHF), single Hartree-Fock (SHF) and double Hartree-Fock (DHF). Surprisingly, they found very little contribution from the non Hartree-Fock diagrams -these are the only ones where the tensor force contributes. For $A = 15$, there was a near cancellation of the (NHF) 1 particle-2 hole and 2 particle-3 hole diagrams. The Hartree-Fock diagrams gave a more substantial contribution. Just to give one example, in the non-relativistic calculation with Bonn A the lowest-order spin-orbit splitting was 4.17 MeV and the contributions of the $1p - 2h$ and $2p-3h$ NHF diagrams were respectively 0.53 MeV and -0.52 MeV (near cancellation). The SHF and DHF contributions were 2.25 MeV and 0.37 MeV respectively. This leads to a final energy splitting of 6.80 MeV.

In the above calculation, the results were given for the whole interaction. In the present work, we will investigate the role of the separate contributions of the central, tensor and spin-orbit interactions as we extend the model space beyond one major shell. To do so, we shall use the simplified (x, y) interaction of Zheng and Zamick [5]which has the form

$$V(r) = V_c(r) + x \cdot V_{s.o.} + y \cdot V_t \tag{1}$$

where $s.o.$ stands for the two-body spin-orbit interaction, t for the tensor interaction, and $V_c(r)$ is everything else, especially the (spin-dependent) central interaction. A good fit to Bonn A matrix elements (from a free G-matrix) is obtained with $x = 1,\ y = 1$. We can study the effects of the spin-orbit and tensor inetractions by varying x and y. More dtails about the interaction are given in reference [5].

Furthermore, we employ the alternative approach of shell model diagonalization in large spaces, rather than use perturbation theory [4]. The OXBASH program that we use [6] automaticaly removes spurious states using the Gloeckner-Lawson technique [7].

II. RESULTS

A. (a) The $A = 5$ System

We shall first give results for the energy splitting $\Delta E = E(1/2^-) - E(3/2^-)$ for the (x, y) interaction in which the two-body spin-orbit interaction is turned off. We give the results for various values of the tensor interaction. We have three model spaces: 0 $\hbar\omega$, (0+2) $\hbar\omega$ and (0+2+4) $\hbar\omega$ corresponding to excitation energies from the valence space. Thus, 0 $\hbar\omega$ corresponds to the case where we have a closed $0s$ shell and the valence particle is in $0p_{3/2}$ or $0p_{1/2}$. For (0+2) $\hbar\omega$ we have the above valence configuration plus all 2 $\hbar\omega$ excitations, etc... We can loosely call ΔE the effective spin-orbit splitting (ESO). But before discussing these results, we shall first present results for the ($x = 1$, $y = 1$) case. Here, the values of ΔE in the 0, (0+2) and (0+2+4) $\hbar\omega$ spaces are 3.375 MeV, 2.224 MeV, and 2.028 MeV, respectively. Thus, in higher order, we get a substantial reduction of the effective spin-orbit splitting for $A = 5$. What is the cause of this reduction? Is it the two-body tensor interaction in play or the two-body spin-orbit interaction?

We see the effects of the tensor interaction in Table I. For $x = 0$, $y = 0$, there is *no* 'spin-orbit' splitting in any of the model spaces. This means that a central interaction, indeed a *spin-dependent* central interaction, cannot induce an efective spin-orbit splitting in higher perturbation theory. Also note that, in the 0 $\hbar\omega$ space, the ESO is zero when $x = 0$. In lowest order, the tensor interaction also does not give any ESO for a closed LS shell plus or minus one particle. As we vary y (keeping $x = 0$), we see an approximate quadratic rise in the effective spin-orbit splitting -in fact, the rise is a bit faster than quadratic in y. The ESO is of the correct sign. However, for the normal free- space tensor strength $y = 1$ the ESO is very small. In the three model spaces of increasing size, the values of ESO obtained are 0, 0.177 MeV and 0.138 MeV. Only for three times the strength of the normal tensor strength (*i.e.* $y = 3$) do we start to get values of ESO which are comparable to what one gets for $x = 1$. The values for $x = 0$ $y = 3$ are 0, 2.148 and 1.842 MeV, whilst for $x = 1$ $y = 1$ they are 3.375, 2.224 and 2.028 MeV.

In Table II, we study the effects of varying the spin-orbit strength in the absence of the tensor interaction. In the 0 $\hbar\omega$ space, the effective spin-orbit splitting ESO varies linearly with x. We thus see how the one-body spin-orbit interaction comes from the two-body spin-orbit interaction in this space. Interestingly, in the higher spaces the ESO also varies very close to linearly with x, the strength of the two-body spin-orbit interaction.

Perhaps the most important result of Table II is that there is a substantial decrease in the spin-orbit interaction as one goes to higher orders. For eample, in the 0, (0+2) and (0+2+4) $\hbar\omega$ spaces the values of ESO for $x = 1$ $(y = 0)$ are 3.375, 1.987 and 1.860 MeV respectively. While there has been some discussion of the enhancement of the spin-orbit interaction for $A = 5$ due to second-order tensor effects [2], we are not aware of any discussion of the spin-orbit interaction in higher order.

Since the change of the spin-orbit interaction as one goes from 0 to (0+2) $\hbar\omega$ space is also linear in x, it must be that the dominant second-order perturbation theory terms are ones in which one of the interactions is spin-orbit whilst the other is central.

We see the combined effects of the spin-orbit and tensor interactions by comparing the $x = 1,\ y = 1$ case (see Table I) with $x = 1,\ y = 0$. In the 0 $\hbar\omega$ space, the ESO's are the same: 3.375 MeV. In the (0+2) $\hbar\omega$ space the values are respectively 2.224 MeV and 1.989 MeV. The decrease in the $x = 1$ $y = 1$ case is not as large as in the $x = 1$ $y = 0$ case because in the former one the tensor interaction is acting so as to make ESO bigger, whilst the spin-orbit interaction in higher order wants to make ESO smaller.

III. THE $A = 15$ SYSTEM

We now consider the $E(3/2_1^-) - E(1/2_1^-)$ splitting in mass 15. In lowest order we have a hole relative to the doubly magic closed shell ^{16}O. The ground state is a $p_{1/2}$ hole, and the excited state is a $p_{3/2}$ hole. We shall consider the 0 $\hbar\omega$ and (0+2) $\hbar\omega$ spaces only, and we show all the results in Table III.

We first comment on the $x = 1$ $y = 1$ case. In contrast to the $A = 5$ case, the ESO here is *larger* in the (0+2) $\hbar\omega$ space than in the 0 $\hbar\omega$ space. We see now that the higher-order effects of the spin-orbit interaction are causing this. For $y = 0$ (no tensor), the ESO gets *larger* in the (0+2) $\hbar\omega$ space than in the 0 $\hbar\omega$ space. In the 0 $\hbar\omega$ space the ESO is linear in x, and in the (0+2) $\hbar\omega$ space it is very nearly linear.

When we vary the tensor interaction with the spin-orbit interaction turned off $(x = 0)$, we get a quadratic behaviour in y, but the effect is very small in itself and has the opposite sign to that of the basic spin-orbit interaction. Recall that for $A = 5$ the second-order tensor effect had the same sign as that of the basic spin-orbit interaction. This is another qualitative difference.

IV. THE A=17 SYSTEM

For $A = 17$, we make a similar table as for $A = 15$, but here the spin-orbit partners are $0d_{5/2}$ and $0d_{3/2}$. We normalize the $0d_{5/2}$ to zero energy, and show not only the $0d_{3/2} - 0d_{5/2}$ splitting, but the $1s_{1/2}$ energy as well. For $x = 1$, $y = 1$, there is hardly any change in the ESO in going from 0 $\hbar\omega$ to (0+2) $\hbar\omega$. The respective values are 5.562 MeV and 5.622 MeV. However, the $1s_{1/2}$ gets depressed more relative to $0d_{5/2}$ by -0.119 MeV and -1.430 MeV, respectively. The behaviour of ESO as a function of the tensor interaction strength y is rather complicated, so we have extended the $x = 0$ calculations in Table IV to $y = 3$ in increments of 0.5. In the (0+2) $\hbar\omega$ space, the value of ESO for $x = 0$ $y = 0$ is of course zero. As we increase y, ESO becomes increasingly negaive (wrong sign) but then there is a turnaround, and for large values of y it becomes positive. The behaviour can be fitted by a formula: ESO $(x = 0) \simeq -0.042y + 0.032y^2$. Note also that for $x = 0$, the splitting $E(0d_{5/2}) - E(1s_{1/2})$ is approximately linear in y with a positive slope.

V. CLOSING REMARKS

We see that the effects of higher-shell admixtures on the single-particle energies, and especially on the effective spin-orbit splitting (ESO) are variable. For $A = 5$, the second-order effects involving the spin-orbit and central interactions cause ESO to decrease, but in $A = 15$ there is a fairly large increase whilst in $A = 17$ there is a very small increase. The decrease in ESO in A=5 and its increase in A=15 reflects that the spin-orbit splittings for the particle states tend to be reduced as compared to those for hole states since the particle states are less localized, as noted in ref. [4]. Our main conclusion here is that the contribution of the second-order tensor interaction to ESO is very small for reasonable strengths of the tensor interaction and can be neglected, for most part. For $A = 5$, the sign of this contribution is the same as that of the two-body spin-orbit interaction, but for $A = 15$ it is of opposite sign, whilst for $A + 17$ there is a sign change from negative to positive as we increase y. Only in 2 $\hbar\omega$ space, for $A = 15$ do we get an enhanced ESO. There is some support for this from experiment. The splitting $E(3/2^-_1) - E(1/2^-_1) = 6.0$ MeV. This is larger than the corresponding $A = 17$ splitting $E(3/2^+_1) - E(5/2^+_1) = 5.1$ MeV. Thus large space calculations are essential in this context to properly account for the differences, in spin-orbit splittings of single particle states above the Fermi energy and of single hole states below the Fermi energy. But in other situations the $p_{1/2} - p_{3/2}$ is smaller than the $d_{3/2} - d_{5/2}$ splitting as inferred from the role of one-body spin-orbit interaction. This is indeed the case between the ESO's for A=5 and A=17.

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TABLES

TABLE I. The Effective Spin-Orbit splitting $ESO = E(1/2^-) - E(3/2^-)$ for $A = 5$ with $x = 0$ (no $two-body$ spin-orbit interaction) and varying y.

x	y	ESO (MeV)		
		0 $\hbar\omega$	(0+2) $\hbar\omega$	(0+2+4) $\hbar\omega$
0	0	0	0	0
0	0.5	0	0.038	0.028
0	1	0	0.177	0.138
0	1.5	0	0.449	0.361
0	2	0	0.870	0.715
0	3	0	2.148	1.842
1	1	3.375	2.224	2.028

TABLE II. The Effective Spin-Orbit splitting $ESO = E(1/2^-) - E(3/2^-)$ for $A = 5$ with $y = 0$ (no tensor interaction) and varying x.

x	y	ESO (MeV)		
		0 $\hbar\omega$	(0+2) $\hbar\omega$	(0+2+4) $\hbar\omega$
0	0	0	0	0
0.5	0	1.687	1.010	0.944
1	0	3.375	1.989	1.860
1.5	0	5.062	2.945	2.752

TABLE III. The $3/2^- - 1/2^-$ splitting in $A = 15$ with various x and y combinations.

x	y	$ESO\ (MeV)$	
		$0\ \hbar\omega$	(0+2) $\hbar\omega$
0	0	0	0
0	0.5	0	-0.002
0	1	0	-0.009
0	1.5	0	-0.019
0.5	0	2.531	3.026
1	0	5.062	6.008
1.5	0	7.593	8.934
1	1	5.063	5.679

TABLE IV. The $3/2^+ - 5/2^+$ splitting in $A = 17$, as well as the $1s_{1/2}$ energy (relative to $0d_{5/2}$ for various x and y combinations.

x	y	$0\ \hbar\omega$		(0+2) $\hbar\omega$	
x	y	ESO	$E(1s_{1/2})$	ESO	$E(1s_{1/2})$
0	0	0	-2.343	0	-3.853
0	0.5	0	-2.343	-0.005	-3.806
0	1	0	-2.343	-0.010	-3.661
0	1.5	0	-2.343	-0.004	-3.419
0	2	0	-2.343	0.020	-3.085
0	2.5	0	-2.343	0.078	-2.671
0	3	0	-2.343	0.160	-2.195
0.5	0	2.782	-1.231	2.849	-2.723
1	0	5.562	-0.119	5.689	-1.618
1.5	0	8.344	0.994	8.512	-0.544
1	1	5.562	-0.119	5.662	-1.430